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Derivation of the Lamb Shift from an Effective Hamiltonian in Non-relativistic Quantum Electrodynamics

By

Asao Arai*

Abstract

Some aspects of spectral analysis of an effective Hamiltonian in non-relativistic quantum electrodynamics are reviewed. The Lamb shift of a hydrogen-like atom is derived as the lowest order approximation (in the fine structure constant) of an energy level shift of the effective Hamiltonian.

§ 1. Introduction

This paper is a review of some results obtained in [7], in which spectral analysis is made on an effective Hamiltonian in non-relativistic quantum electrodynamics (QED), a quantum theory of non-relativistic charged particles interacting with the quantum radiation field (a quantum field theoretical version of a vector potential in classical electrodynamics). In this introduction, we explain some physical backgrounds behind the work [7].

A hydrogen-like atom is an atom consisting of one electron, whose electric charge is $-e < 0$, and a nucleus with electric charge $Ze > 0$, where Z is a natural number (the case $Z = 1$ is the usual hydrogen atom). As is well known, if the nucleus is fixed at the origin of the 3-dimensional Euclidean vector space $\mathbb{R}^3 = \{\mathbf{x} = (x_1, x_2, x_3) | x_j \in \mathbb{R}, j = 1, 2, 3\}$ and, as the potential acting on the electron at the position $\mathbf{x} \in \mathbb{R}^3$, one takes into

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account only the electric Coulomb potential¹ $-Ze^2/4\pi|\mathbf{x}|$ from the nucleus, then a quantum mechanical Hamiltonian describing the hydrogen-like atom is given by the Schrödinger operator

$$(1.1) \quad H_{\text{hyd}} = -\frac{\hbar^2}{2m_e}\Delta - \frac{\gamma}{|\mathbf{x}|}$$

acting on $L^2(\mathbb{R}^3)$, the Hilbert space of equivalence classes of complex-valued functions square integrable on \mathbb{R}^3 with respect to the 3-dimensional Lebesgue measure, where $\hbar := h/2\pi$ (h is the Planck constant), $m_e > 0$ is the electron mass, Δ is the generalized Laplacian on $L^2(\mathbb{R}^3)$, and

$$\gamma := \frac{Ze^2}{4\pi}.$$

Indeed, H_{hyd} is self-adjoint with domain $D(H_{\text{hyd}}) = D(\Delta)$ —for a linear operator A on a Hilbert space, $D(A)$ denotes the domain of A —and the spectrum of H_{hyd} , denoted $\sigma(H_{\text{hyd}})$, is found to be

$$(1.2) \quad \sigma(H_{\text{hyd}}) = \{E_n\}_{n=1}^{\infty} \cup [0, \infty)$$

with

$$(1.3) \quad E_n = -\frac{1}{2} \frac{m_e \gamma^2}{\hbar^2} \frac{1}{n^2}, \quad n = 1, 2, 3, \dots,$$

where each eigenvalue E_n is degenerate with multiplicity n^2 (e.g., [6, §2.3.5a] and [6, Lemma 5.22, footnote 12]). These eigenvalues explain very well the so-called principal energy levels of the hydrogen-like atom (Fig.1(a)), but do not show the finer structures of the energy spectrum (Fig.1(b)), which may be regarded as splittings of the degeneracy of E_n 's.

It turns out that the finer structures of the hydrogen-like atom can be explained by the Dirac operator

$$D_{\text{hyd}} := -i\hbar c \sum_{k=1}^3 \alpha_k D_k + m_e c^2 \beta - \frac{\gamma}{|\mathbf{x}|},$$

acting on $\oplus^4 L^2(\mathbb{R}^3)$ (the four direct sum of $L^2(\mathbb{R}^3)$), where $c > 0$ is the speed of light in the vacuum, D_k is the generalized partial differential operator in the variable x_k , and α_k, β are 4×4 Hermitian matrices satisfying the following anti-commutation relations (δ_{kl} denotes the Kronecker delta):

$$\alpha_k \alpha_l + \alpha_l \alpha_k = 2\delta_{kl}, \quad \alpha_k \beta + \beta \alpha_k = 0, \quad \beta^2 = 1 \quad (k, l = 1, 2, 3).$$

¹The electromagnetic system of units which we use in the present paper is the rationalized CGS Gauss unit system with the dielectric constant in the vacuum equal to 1.

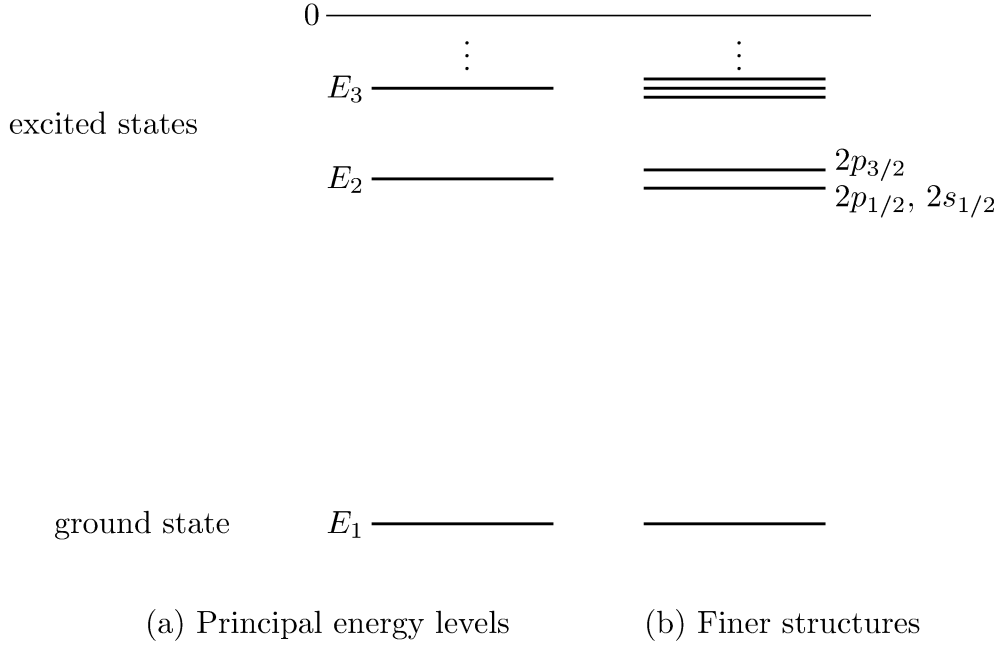


Figure 1. Energy spectrum of a hydrogen-like atom

The operator D_{hyd} is a relativistic version of H_{hyd} [15].

It is shown [15, §7.4] that the discrete spectrum $\sigma_{\text{disc}}(D_{\text{hyd}})$ of D_{hyd} is given by

$$\sigma_{\text{disc}}(D_{\text{hyd}}) = \{E_{n,j}\}_{n,j}$$

with

$$E_{n,j} = \frac{m_e c^2}{\sqrt{1 + \frac{1}{\hbar^2 c^2} \left(\frac{\gamma}{n - \left(j + \frac{1}{2}\right) + \sqrt{\left(j + \frac{1}{2}\right)^2 - \frac{\gamma^2}{\hbar^2 c^2}}} \right)^2}}, \quad n = 1, 2, \dots,$$

where j ($1/2 \leq j \leq n - 1/2$) is the total angular momentum of the electron, being related to the orbital angular momentum $\ell = 0, 1, \dots$ by $j = \ell \pm 1/2$ ($\pm 1/2$ are the possible values of the spin of the electron), and the condition $\gamma/\hbar c < 1$ is assumed.

It is easy to see that $E_{n,j}$ is monotone increasing in n and that, for each n ,

$$E_{n,j} < E_{n,j+1}.$$

Note also that the non-relativistic limit² $c \rightarrow \infty$ of $E_{n,j} - m_e c^2$ gives E_n :

$$\lim_{c \rightarrow \infty} (E_{n,j} - m_e c^2) = E_n, \quad n = 1, 2, \dots$$

For each $n = 1, 2, \dots$, the state with energy eigenvalue $E_{n,j}$ and angular momentum $\ell = 0, 1, 2, 3, 4, \dots$ is respectively labeled as nx_j with $x = s, p, d, f, g, \dots$:

principal number	state
$n = 1$	$1s_{1/2}$
$n = 2$	$(2s_{1/2}, 2p_{1/2}), \quad 2p_{3/2}$
$n = 3$	$(3s_{1/2}, 3p_{1/2}), \quad (3p_{3/2}, 3d_{3/2}), \quad 3d_{5/2}$
\vdots	\vdots

Here the states in each round bracket are degenerate. For example, the states $2s_{1/2}$ and $2p_{1/2}$ are degenerate with energy $E_{2,1/2}$. The energy levels $E_{2,1/2}$ and $E_{2,3/2}$ are very near with $E_{2,1/2} < E_{2,3/2}$. Hence these energy levels subtracted by $m_e c^2$ may be regarded as a splitting of the second principal energy level E_2 in the non-relativistic theory. It is known that the energy levels $\{E_{n,j} - m_e c^2\}_{n,j}$ gives a good agreement with experimental data (Fig.1(b)).

In 1947, however, Lamb and Retherford [12] experimentally observed that there is a very small difference between the energies of the states $2s_{1/2}$ and $2p_{1/2}$ with the former being higher than the latter (Fig.2). This difference is called the *Lamb shift*. Thus the Dirac theory breaks down in this respect.

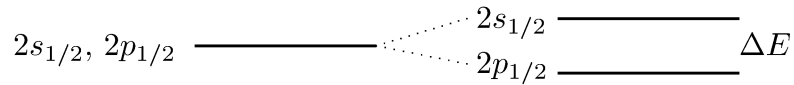


Figure 2. ΔE =Lamb shift

It was Bethe [8] who first explained the Lamb shift using non-relativistic QED. He considered the Lamb shift as an energy shift caused by the interaction of the electron with the quantum radiation field. In his calculation, which is based on the standard heuristic perturbation theory, the mass renormalization of the electron is one of the essential prescriptions. On the other hand, Welton [16] gave another method to explain the Lamb

²In a non-relativistic theory, the kinetic energy of a rest particle is zero. Hence, in taking the non-relativistic limit of an energy in a relativistic theory, one must subtract the rest energy $m_e c^2$ from it.

shift using non-relativistic QED: He infers that the interaction of the electron with the quantum radiation field may give rise to fluctuations of the position of the electron and these fluctuations may change the Coulomb potential so that the energy level shift such as the Lamb shift may occur. With this physical intuition, he derived the Lamb shift heuristically and perturbatively. After the work of Bethe and Welton, perturbative calculations of the Lamb shift using relativistic QED with prescription of renormalizations have been made, giving amazingly good agreements with the experimental result (see, e.g., [11]). However a mathematically rigorous construction of relativistic QED (existence of full relativistic QED) is still open as one of most important and challenging problems in modern mathematical physics. On the other hand, non-relativistic QED allows one to analyze it in a mathematically rigorous way [1, 2, 3] (for a review of recent developments of non-relativistic QED, see, e.g., [10])

Motivated by finding a mathematically general theory behind Welton's heuristic arguments made in [16], the present author developed in the paper [4] an abstract theory of scaling limit for self-adjoint operators on a Hilbert space and applied it to one-particle non-relativistic QED (a quantum mechanical model of a non-relativistic charged particle interacting with the quantum radiation field; a variant of the Pauli-Fierz model [13]) to obtain an effective Hamiltonian of the whole quantum system. This result is the starting point of the present review. Thus we next explain it in some detail.

§ 2. A Model in Non-relativistic QED and its Scaling Limit

For mathematical generality, the non-relativistic charged particle is assumed to appear in the d -dimensional Euclidean vector space \mathbb{R}^d with $d \geq 2$, so that the Hilbert space of state vectors for the charged particle is taken to be $L^2(\mathbb{R}^d)$. We consider the situation where the charged particle is under the influence of a scalar potential $V : \mathbb{R}^d \rightarrow \mathbb{R}$ (Borel measurable). Then the non-relativistic Hamiltonian of the charged particle with mass $m > 0$ is given by the Schrödinger operator

$$(2.1) \quad H(m) := -\frac{\hbar^2}{2m} \Delta + V.$$

On the other hand, the Hilbert space of state vectors of a photon is given by

$$\mathcal{H}_{\text{ph}} := \oplus^{d-1} L^2(\mathbb{R}^d),$$

the $(d-1)$ -direct sum of $L^2(\mathbb{R}^d)$, where the number $(d-1)$ in the present context means the freedom of polarization of a photon and \mathbb{R}^d here denotes the space of wave number vectors of a photon. Then the Hilbert space of state vectors for the quantum radiation

field is given by the boson Fock space

$$\begin{aligned}\mathcal{F}_{\text{rad}} &:= \oplus_{n=0}^{\infty} \otimes_s^n \mathcal{H}_{\text{ph}} \\ &= \left\{ \Psi = \{\Psi^{(n)}\}_{n=0}^{\infty} \mid \Psi^{(n)} \in \otimes_s^n \mathcal{H}_{\text{ph}}, n \geq 0, \sum_{n=0}^{\infty} \|\Psi^{(n)}\|^2 < \infty \right\}\end{aligned}$$

over \mathcal{H}_{ph} , where $\otimes_s^n \mathcal{H}_{\text{ph}}$ denotes the n -fold symmetric tensor product of \mathcal{H}_{ph} with $\otimes_s^0 \mathcal{H}_{\text{ph}} := \mathbb{C}$ (the set of complex numbers) and $\|\Psi^{(n)}\|$ denotes the norm of $\Psi^{(n)}$.

As is easily shown, $\otimes_s^n \mathcal{H}_{\text{ph}}$ is identified with the Hilbert space of square integrable functions $\psi^{(n)}((\mathbf{k}_1, s_1), (\mathbf{k}_2, s_2), \dots, (\mathbf{k}_n, s_n))$ on $(\mathbb{R}^d \times \{1, \dots, d-1\})^n$ ($\mathbf{k}_j \in \mathbb{R}^d, s_k \in \{1, \dots, d-1\}$) which are totally symmetric in the variables $(\mathbf{k}_1, s_1), (\mathbf{k}_2, s_2), \dots, (\mathbf{k}_n, s_n)$, where the isomorphism comes from the correspondence

$$S_n(\otimes_{j=1}^n \psi_j) \rightarrow \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \psi_{\sigma(1)}(\mathbf{k}_1, s_1) \cdots \psi_{\sigma(n)}(\mathbf{k}_n, s_n), \quad \psi_j = (\psi_j(\cdot, s))_{s=1}^{d-1} \in \mathcal{H}_{\text{ph}}$$

with S_n being the symmetrization operator on $\otimes^n \mathcal{H}_{\text{ph}}$ and \mathfrak{S}_n denotes the symmetry group of n -th order. We use this identification.

In the physical case $d = 3$, the energy of a photon with wave number vector $\mathbf{k} \in \mathbb{R}^3$ is given by $\hbar c|\mathbf{k}|$ (by Planck-Einstein-de Broglie relation, $\hbar\mathbf{k}$ is the momentum of the photon with wave number vector \mathbf{k}). Thus, in the case of general dimensions d , we assume that the energy of a photon with wave number vector $\mathbf{k} \in \mathbb{R}^3$ is given by $\hbar c\omega(\mathbf{k})$ with a function $\omega : \mathbb{R}^d \rightarrow [0, \infty)$ such that $0 < \omega(\mathbf{k}) < \infty$ for a.e. (almost everywhere) $\mathbf{k} \in \mathbb{R}^d$ with respect to the Lebesgue measure on \mathbb{R}^d . Then the free Hamiltonian of the quantum radiation field is defined by

$$H_{\text{rad}} := \oplus_{n=0}^{\infty} \hbar c \omega^{(n)},$$

where $\omega^{(0)} := 0$ and $\omega^{(n)}$ is the multiplication operator by the function

$$\omega^{(n)}(\mathbf{k}_1, \dots, \mathbf{k}_n) := \sum_{j=1}^n \omega(\mathbf{k}_j)$$

on $(\mathbb{R}^d \times \{1, \dots, d-1\})^n$.

For each $f \in \mathcal{H}_{\text{ph}}$, there exists a densely defined closed linear operator $a(f)$ on \mathcal{F}_{rad} , called the photon annihilation operator with test vector f , such that its adjoint $a(f)^*$ takes the form

$$(a(f)^* \Psi)^{(0)} = 0, \quad (a(f)^* \Psi)^{(n)} = S_n(f \otimes \Psi^{(n-1)}), \quad \Psi = \{\Psi^{(n)}\}_{n=0}^{\infty} \in D(a(f)^*), n \geq 1$$

(for more details, see [5, Chapter 10]). The operators $a(f)$ and $a(g)^*$ ($f, g \in \mathcal{H}_{\text{ph}}$) satisfy the commutation relations—canonical commutation relations (CCR)—

$$\begin{aligned}[a(f), a(g)^*] &= \langle f, g \rangle, \\ [a(f), a(g)] &= 0, \quad [a(f)^*, a(g)^*] = 0\end{aligned}$$

on the subspace

$$\mathcal{F}_{\text{rad},0} := \{\Psi = \{\Psi^{(n)}\}_{n=0}^\infty \in \mathcal{F}_{\text{rad}} | \exists n_0 \text{ such that } \Psi^{(n)} = 0, \forall n \geq n_0\},$$

where $[A, B] := AB - BA$ and $\langle \cdot, \cdot \rangle$ denotes inner product. Thus the set $\{a(f), a(f)^* | f \in \mathcal{H}_{\text{ph}}\}$ gives a representation of the CCR indexed by \mathcal{H}_{ph} .

For a.e. $\mathbf{k} \in \mathbb{R}^d$, there exists an orthonormal system $\{\mathbf{e}^{(s)}(\mathbf{k})\}_{s=1}^{d-1}$ of \mathbb{R}^d such that each vector $\mathbf{e}^{(s)}(\mathbf{k}) = (e_1^{(s)}(\mathbf{k}), \dots, e_d^{(s)}(\mathbf{k}))$ is orthogonal to \mathbf{k} .

Let ρ be a real distribution on \mathbb{R}^d such that its Fourier transform $\hat{\rho}$ is a function satisfying

$$\frac{\hat{\rho}}{\omega^a} \in L^2(\mathbb{R}^d) \setminus \{0\}, \quad a = \frac{3}{2}, \frac{1}{2}.$$

Then the quantum radiation field $A(\rho) := (A_1(\rho), \dots, A_d(\rho))$ smeared with ρ is defined by

$$A_j(\rho) = \frac{\sqrt{\hbar c}}{\sqrt{2}} \left\{ a \left(\frac{\hat{\rho}}{\sqrt{\omega}} e_j \right)^* + a \left(\frac{\hat{\rho}}{\sqrt{\omega}} e_j \right) \right\}, \quad j = 1, \dots, d,$$

where $e_j : \mathbb{R}^d \rightarrow \mathbb{R}^{d-1}$, $e_j(\mathbf{k}) := (e_j^{(1)}(\mathbf{k}), \dots, e_j^{(d-1)}(\mathbf{k}))$, a.e. $\mathbf{k} \in \mathbb{R}^d$. We remark that, for the definition of $A_j(\rho)$ itself, condition $\hat{\rho}/\sqrt{\omega} \in L^2(\mathbb{R}^d)$ is sufficient. The additional condition $\hat{\rho}/\omega^{3/2} \in L^2(\mathbb{R}^d)$ is needed in the development below.

The Hilbert space \mathfrak{H} of state vectors of the quantum system under consideration is given by

$$\mathfrak{H} = L^2(\mathbb{R}^d) \otimes \mathcal{F}_{\text{rad}}.$$

The Hamiltonian of our model is of the following form:

$$H_{\text{NR}} = H(m_0) \otimes I + I \otimes H_{\text{rad}} + H_{\text{I}}(\rho, m_0)$$

with

$$H_{\text{I}}(\rho, m_0) := -\frac{q}{m_0 c} \sum_{j=1}^d p_j \otimes A_j(\rho),$$

where $m_0 > 0$ is the “bare” mass of the particle (the mass of the particle before going into the interaction with the quantum radiation field), $q \in \mathbb{R}$ and $p_j := -i\hbar D_j$ denote respectively the electric charge and the momentum operator of the particle. The operator $H_{\text{I}}(\rho, m_0)$ describes an interaction of the charged particle with the quantum radiation field. In this context, the function $\hat{\rho}$ plays a role of momentum cutoff for photons interacting with the particle.

To draw from the Hamiltonian H_{NR} observable effects that the quantum field may give rise to the quantum particle, we consider a scaling limit of H_{NR} . Thus we introduce the following scaled Hamiltonian:

$$H_{\text{NR}}(\kappa) := H(m(\kappa)) \otimes I + \kappa I \otimes H_{\text{rad}} + \kappa H_{\text{I}}(\rho, m), \quad \kappa > 0,$$

where $m > 0$ is the observed mass of the particle and

$$m(\kappa) := \frac{m}{1 + 4\kappa\lambda_q m}$$

with

$$\lambda_q := \frac{(d-1)}{4d} \left(\frac{\hbar}{mc} \right)^2 \frac{q^2}{\hbar^2} \int_{\mathbb{R}^d} \frac{|\hat{\rho}(\mathbf{k})|^2}{\omega(\mathbf{k})^3} d\mathbf{k}$$

Under the assumption that V is infinitesimally small with respect to $-\Delta$, the operator $H_{\text{NR}}(\kappa)$ is self-adjoint and bounded below [4, Lemma 3.1].

Remark 2.1. The scaled Hamiltonian $H_{\text{NR}}(\kappa)$ is obtained by the scaling $c \rightarrow \kappa c$ and $q \rightarrow \kappa^{3/2} q$ in H_{NR} with $H(m_0)$ and $H_{\text{I}}(\rho, m_0)$ replaced by $H(m(1))$ and $H_{\text{I}}(\rho, m)$ respectively. Replacing m_0 with $m(\kappa)$ is called a mass renormalization³. We want to emphasize that the mass renormalization makes the Hamiltonian bounded below (under the condition that $H(m)$ is bounded below) [4, Lemma 3.1].

A scaling limit of the original Pauli-Fierz model with dipole approximation is discussed in [9] (see also [10]).

The vector

$$\Omega_0 := \{1, 0, 0, \dots\} \in \mathcal{F}_{\text{rad}} \quad (\Omega^{(0)} = 1, \Omega^{(n)} = 0, n \geq 1)$$

is called the Fock vacuum in \mathcal{F}_{rad} . We denote by P_0 the orthogonal projection onto the 1-dimensional subspace $\{\alpha\Omega_0 | \alpha \in \mathbb{C}\}$ spanned by Ω_0 .

It is shown that the operator

$$T := \frac{iq}{mc} \sum_{j=1}^d p_j \otimes \frac{1}{\sqrt{2\hbar c}} \left\{ a \left(\frac{\hat{\rho}}{\omega^{3/2}} e_j \right)^* - a \left(\frac{\hat{\rho}}{\omega^{3/2}} e_j \right) \right\}$$

is essentially self-adjoint. We denote its closure by \overline{T} .

The following theorem is proved [4, Theorem 3.4]:

Theorem 2.2. Suppose that V satisfies the following two conditions:

(V.1) $D(\Delta) \subset D(V)$ and, for all $a > 0$, $V(-\Delta + a)^{-1}$ is bounded with $\lim_{a \rightarrow \infty} \|V(-\Delta + a)^{-1}\| = 0$.

³Strictly speaking, one should replace m_0 in $H_{\text{I}}(\rho, m_0)$ with $m(\kappa)$ too. But, since

$$H_{\text{I}}(\rho, m(\kappa)) = H_{\text{I}}(\rho, m) - \frac{4\kappa q \lambda_q}{c} \sum_{j=1}^d p_j \otimes A_j(\rho).$$

and the second term on the right hand side is of the third order in q , one may take into account only the first term on the right hand side as a primary approximation in a perturbative sense.

(V.2) For all $t > 0$, $\int_{\mathbb{R}^d} e^{-t|\mathbf{y}|^2} |V(\mathbf{y})| d\mathbf{y} < \infty$.

Then, for all $z \in \mathbb{C} \setminus \mathbb{R}$,

$$\text{s-}\lim_{\kappa \rightarrow \infty} (H_{\text{NR}}(\kappa) - z)^{-1} = e^{-i\bar{T}} ((H_{\text{eff}} - z)^{-1} \otimes P_0) e^{i\bar{T}},$$

where s-lim means strong limit and

$$(2.2) \quad H_{\text{eff}} := -\frac{\hbar^2}{2m} \Delta + V_{\text{eff}}$$

with

$$(2.3) \quad V_{\text{eff}}(\mathbf{x}) := \frac{1}{(4\pi\lambda_q)^{d/2}} \int_{\mathbb{R}^d} e^{-|\mathbf{x}-\mathbf{y}|^2/4\lambda_q} V(\mathbf{y}) d\mathbf{y}, \quad \mathbf{x} \in \mathbb{R}^d.$$

Remark 2.3. Under condition (V.1), V is infinitesimally small with respect to $-\Delta$ and hence $H(m_0)$ is self-adjoint and bounded below for all $m_0 > 0$. Moreover, under conditions (V.1) and (V.2), V_{eff} is infinitesimally small with respect to $-\Delta$ and hence H_{eff} is self-adjoint and bounded below (see [4, §III, B]).

Theorem 2.2 may be physically interpreted as follows: the limiting system as $\kappa \rightarrow \infty$ restricted to the subspace $L^2(\mathbb{R}^3) \otimes \{\alpha e^{-i\bar{T}} \Omega_0 | \alpha \in \mathbb{C}\}$ is equivalent to the particle system whose Hamiltonian is H_{eff} . Therefore H_{eff} may include observable effects of the original interacting system through V_{eff} . In this sense, we call V_{eff} an effective potential for the particle system and, correspondingly to this, we call H_{eff} an effective Hamiltonian of the particle interacting with the quantum radiation field.

To see if the effective Hamiltonian H_{eff} really explains some observable effects, one has to investigate the spectral properties of it. This was the main motivation of the paper [7]. In what follows, we concentrate our attention on this aspect.

§ 3. Elementary Properties of the Effective Hamiltonian

It is obvious that $q \rightarrow 0$ if and only if $\lambda_q \rightarrow 0$. Hence we replace λ_q by a parameter $\lambda > 0$ and regard λ as a perturbation parameter, where the limit $\lambda \downarrow 0$ corresponds to the unperturbed case. Thus we consider the effective Hamiltonian in the form

$$(3.1) \quad H_\lambda := -\frac{\hbar^2}{2m} \Delta + V_\lambda, \quad \lambda > 0,$$

with

$$(3.2) \quad V_\lambda(\mathbf{x}) := \frac{1}{(4\pi\lambda)^{d/2}} \int_{\mathbb{R}^d} e^{-|\mathbf{x}-\mathbf{y}|^2/4\lambda} V(\mathbf{y}) d\mathbf{y}.$$

As for V , we assume only that

$$(3.3) \quad \int_{\mathbb{R}^d} e^{-t|\mathbf{y}|^2} |V(\mathbf{y})| d\mathbf{y} < \infty, \quad \forall t > 0.$$

We have

$$(3.4) \quad H_{\text{eff}} = H_{\lambda_q}.$$

Remark 3.1. If $V \in L^p(\mathbb{R}^d)$ for some $1 \leq p \leq \infty$, then (3.3) is satisfied.

Note that V_λ is the convolution of V and the Gaussian function

$$(3.5) \quad G_\lambda(\mathbf{x}) := \frac{1}{(4\pi\lambda)^{d/2}} e^{-\mathbf{x}^2/4\lambda}, \quad \mathbf{x} \in \mathbb{R}^d,$$

i.e.,

$$(3.6) \quad V_\lambda = G_\lambda * V.$$

In other words, V_λ is the Gauss transform of V with the Gaussian function G_λ . This structure may be suggestive, because the function $G_\lambda(\mathbf{x} - \mathbf{y})$ of \mathbf{x} and \mathbf{y} is the integral kernel of the heat semi-group $\{e^{\lambda\Delta}\}_{\lambda>0}$ on $L^2(\mathbb{R}^d)$ (the heat kernel).

The effective potential V_λ is a perturbation of V in the following senses:

- (i) If V is continuous and $\sup_{\mathbf{x} \in \mathbb{R}^d} |V(\mathbf{x})| e^{-c|\mathbf{x}|^\alpha} < \infty$ for some $c > 0$ and $\alpha \in [0, 2)$, then

$$\lim_{\lambda \downarrow 0} V_\lambda(\mathbf{x}) = V(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d.$$

- (ii) If $V \in L^2(\mathbb{R}^d)$, then

$$V_\lambda = e^{\lambda\Delta} V \in L^2(\mathbb{R}^d).$$

and hence $\lim_{\lambda \rightarrow 0} \|V_\lambda - V\|_{L^2(\mathbb{R}^d)} = 0$ holds⁴.

- (iii) If $V \in L^p(\mathbb{R}^d)$ for some $p \in [1, \infty)$, then $V_\lambda \in L^p(\mathbb{R}^d)$ and

$$\lim_{\lambda \rightarrow 0} \|V_\lambda - V\|_{L^p(\mathbb{R}^d)} = 0.$$

- (iv) If $V \in L^\infty(\mathbb{R}^d)$ and V is uniformly continuous on \mathbb{R}^d , then $V_\lambda \in L^\infty(\mathbb{R}^d)$ and

$$\lim_{\lambda \rightarrow 0} \|V_\lambda - V\|_{L^\infty(\mathbb{R}^d)} = 0.$$

⁴For $p \in [1, \infty]$, $\|\cdot\|_{L^p(\mathbb{R}^d)}$ denotes the norm of $L^p(\mathbb{R}^d)$.

Thus, from a perturbation theoretical point of view, it is natural to write

$$(3.7) \quad H_\lambda = H_0 + W_\lambda$$

with

$$(3.8) \quad H_0 := H(m) = -\frac{\hbar^2}{2m}\Delta + V,$$

$$(3.9) \quad W_\lambda := V_\lambda - V.$$

However, we want to emphasize that H_λ is not necessarily a regular perturbation of H in the sense of [14, §XII.2]. Even in that case, the order of the perturbation may be infinite.

One can analyze general aspects of spectra of H_λ [7]. But, here, we restrict ourselves to the case where V is a spherically symmetric function on \mathbb{R}^3 .

§ 4. Spectral Properties of H_λ with a Spherically Symmetric Potential V on \mathbb{R}^3

We consider the case where $d = 3$ and V is given by the following form:

$$(4.1) \quad V(\mathbf{x}) = \frac{u(|\mathbf{x}|)}{|\mathbf{x}|}, \quad \mathbf{x} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$$

with $u : [0, \infty) \rightarrow \mathbb{R}$ being *bounded and continuously differentiable on $[0, \infty)$ with the derivative u' bounded on $[0, \infty)$* . Note that V has singularity at $\mathbf{x} = \mathbf{0}$ if $u(\mathbf{0}) \neq 0$. It is easy to see that this V satisfies condition (3.3). By direct computations, one sees that the effective potential V_λ in the present case takes the form

$$(4.2) \quad V_\lambda(\mathbf{x}) = \frac{e^{-|\mathbf{x}|^2/4\lambda}}{\sqrt{\pi\lambda}|\mathbf{x}|} \int_0^\infty e^{-r^2/4\lambda} u(r) \sinh \frac{|\mathbf{x}|r}{2\lambda} dr.$$

In particular, V_λ also is spherically symmetric⁵.

A basic result on the spectra of H_λ is stated in the next theorem:

Theorem 4.1. Let V be given by (4.1). Then, for all $\lambda \geq 0$, H_λ is self-adjoint with $D(H_\lambda) = D(\Delta)$ and bounded below. Moreover

$$\sigma_{\text{ess}}(H_\lambda) = [0, \infty),$$

where $\sigma_{\text{ess}}(\cdot)$ denotes essential spectrum, and, if there exists an $r_0 > 0$ such that $\sup_{r \geq r_0} u(r) < 0$, then the discrete spectrum $\sigma_{\text{disc}}(H_\lambda)$ is infinite.

⁵It is an easy exercise to show that, if V is spherically symmetric on \mathbb{R}^d , then so is V_λ .

Suppose that H_0 has an isolated eigenvalue $E_0 \in \mathbb{R}$ with finite multiplicity $m(E_0)$ ($1 \leq m(E_0) < \infty$). Let r be a constant satisfying

$$0 < r < \min_{E \in \sigma(H_0) \setminus \{E_0\}} |E - E_0|.$$

Then

$$C_r(E_0) := \{z \in \mathbb{C} \mid |z - E_0| = r\} \subset \rho(H_0),$$

Let

$$n_r := r \sup_{z \in C_r(E_0)} \|(H_0 - z)^{-1}\|, \quad r_\lambda := \sup_{z \in C_r(E_0)} \|W_\lambda(H_0 - z)^{-1}\|.$$

Theorem 4.2. Let $r_\lambda < 1/(1 + n_r)$. Then, H_λ has exactly $m(E_0)$ eigenvalues in the interval $(E_0 - r, E_0 + r)$, counting multiplicities, and $\sigma(H_\lambda) \cap (E_0 - r, E_0 + r)$ consists of only these eigenvalues.

In the case where E_0 is a simple eigenvalue of H , one can obtain more detailed results:

Corollary 4.3. Let $r_\lambda < 1/(1 + n_r)$. Suppose that $m(E_0) = 1$ and Ω_0 is a normalized eigenvector of H with eigenvalue E_0 . Then, H_λ has exactly one simple eigenvalue E_λ in the interval $(E_0 - r, E_0 + r)$ with formula

$$E_\lambda = E_0 + \frac{\langle \Omega_0, W_\lambda \Omega_0 \rangle + \sum_{n=1}^{\infty} S_n(\lambda)}{1 + \sum_{n=1}^{\infty} T_n(\lambda)},$$

where

$$S_n(\lambda) := \frac{(-1)^{n+1}}{2\pi i} \int_{C_r(E_0)} dz \left\langle \Omega_0, [W_\lambda(H - z)^{-1}]^{n+1} \Omega_0 \right\rangle,$$

$$T_n(\lambda) := \frac{(-1)^{n+1}}{2\pi i} \int_{C_r(E_0)} dz \frac{\langle \Omega_0, [W_\lambda(H - z)^{-1}]^n \Omega_0 \rangle}{E_0 - z},$$

and $\sigma(H_\lambda) \cap (E_0 - r, E_0 + r) = \{E_\lambda\}$. Moreover, a normalized eigenvector of H_λ with eigenvalue E_λ is given by

$$\Omega_\lambda = \frac{\Omega_0 + \sum_{n=1}^{\infty} \Omega_{\lambda,n}}{\sqrt{1 + \sum_{n=1}^{\infty} T_n(\lambda)}},$$

where

$$\Omega_{\lambda,n} := \frac{(-1)^{n+1}}{2\pi i} \int_{C_r(E_0)} dz (H - z)^{-1} [W_\lambda(H - z)^{-1}]^n \Omega_0.$$

§ 5. Reductions of H_λ to Closed Subspaces

The Hilbert space $L^2(\mathbb{R}^3)$ has the orthogonal decomposition

$$L^2(\mathbb{R}^3) = \oplus_{\ell=0}^{\infty} \oplus_{s=-\ell}^{\ell} \mathcal{H}_\ell^s$$

with

$$\mathcal{H}_\ell^s = L^2([0, \infty), r^2 dr) \otimes \{\alpha Y_\ell^s | \alpha \in \mathbb{C}\},$$

where Y_ℓ^s is the spherical harmonics with index (ℓ, s) :

$$Y_\ell^s(\theta, \phi) := (-1)^s \sqrt{\frac{(\ell-s)!}{(\ell+s)!}} \sqrt{\frac{2\ell+1}{4\pi}} P_\ell^s(\cos \theta) e^{is\phi},$$

$$\theta \in [0, \pi], \phi \in [0, 2\pi), s = -\ell, -\ell+1, \dots, 0, \dots, \ell-1, \ell$$

with P_ℓ^s being the associated Legendre function:

$$P_\ell^s(x) := (1-x^2)^{s/2} \frac{d^s}{dx^s} \frac{(-1)^\ell}{2^\ell \ell!} \left(\frac{d}{dx} \right)^\ell (1-x^2)^\ell, \quad |x| < 1.$$

We have

$$\int_0^\pi d\theta \int_0^{2\pi} d\phi \sin \theta Y_\ell^s(\theta, \phi)^* Y_{\ell'}^{s'}(\theta, \phi) = \delta_{\ell\ell'} \delta_{ss'}.$$

As we have already seen, V_λ under consideration is spherically symmetric. Hence H_λ is reduced by each \mathcal{H}_ℓ^s . We denote the reduced part of H_λ by $H_\lambda^{\ell,s}$:

$$(H_\lambda^{\ell,s} f \otimes Y_\ell^s)(r, \phi, \theta) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \tilde{V}_\lambda(r) - \frac{\hbar^2}{2m} \frac{2}{r} \frac{d}{dr} \right) f(r) Y_\ell^s(\theta, \phi) \\ + \frac{\ell(\ell+1)}{r^2} f(r) Y_\ell^s(\theta, \phi), \quad f \in C_0^\infty(0, \infty),$$

where $\tilde{V}_\lambda(r) := V_\lambda(\mathbf{x})|_{r=|\mathbf{x}|}$ and $C_0^\infty(0, \infty)$ is the set of infinitely differentiable functions on $(0, \infty)$ with bounded support in $(0, \infty)$.

Corollary 5.1. For each pair (ℓ, s) ($\ell \in \{0\} \cup \mathbb{N}$, $s = -\ell, -\ell+1, \dots, \ell$), Theorem 4.2 and Corollary 4.3 with H_λ replaced by $H_\lambda^{\ell,s}$ hold.

§ 6. Energy Level Shifts in a Hydrogen-like Atom

Now we consider a hydrogen-like atom mentioned in Introduction. Thus we take as an unperturbed Hamiltonian H_0 the Schrödinger operator H_{hyd} defined by (1.1):

$$(6.1) \quad H_{\text{hyd}} = -\frac{\hbar^2}{2m_e} \Delta + V^{(\gamma)}, \quad V^{(\gamma)} := -\frac{\gamma}{|\mathbf{x}|}.$$

The eigenvalue E_n of H_{hyd} (see (1.3)) is a unique simple eigenvalue of the reduced part $H_{\text{hyd}}^{\ell,s}$ of H_{hyd} ($0 \leq \ell \leq n-1$) to the closed subspace \mathcal{H}_ℓ^s with a normalized eigenfunction

$$\psi_{n,\ell,s}(\mathbf{x}) := C_{n,\ell} e^{-\beta_n r/2} (\beta_n r)^\ell L_{n+\ell}^{2\ell+1}(\beta_n r) Y_\ell^s(\theta, \phi),$$

$$r = |\mathbf{x}|, \ell = 0, 1, \dots, n-1,$$

where

$$\beta_n := \frac{2m_e\gamma}{\hbar^2 n},$$

L_n^k ($0 \leq k \leq n$) is the Laguerre associated polynomial with order $n - k$, i.e.,

$$L_n^k(x) = \frac{d^k}{dx^k} L_n(x), \quad x \in \mathbb{R}$$

with $L_n(x)$ being the n -th Laguerre polynomial and

$$C_{n,\ell} := \frac{\beta_n^{3/2} \sqrt{(n-\ell-1)!}}{\sqrt{[(n+\ell)!]^3 2n}}.$$

Applying (4.2) with $u = -\gamma$ (a constant function), the effective potential

$$V_\lambda^{(\gamma)} := G_\lambda * V^{(\gamma)}$$

in the present case is of the form:

$$V_\lambda^{(\gamma)} = V^{(\gamma)} + W_\lambda^{(\gamma)}$$

with

$$W_\lambda^{(\gamma)}(\mathbf{x}) := \frac{2\gamma}{\sqrt{\pi}|\mathbf{x}|} \text{Erfc}(|\mathbf{x}|/2\sqrt{\lambda}),$$

where $\text{Erfc} : \mathbb{R} \rightarrow [0, \infty)$ is the Gauss error function:

$$\text{Erfc}(x) := \int_x^\infty e^{-y^2} dy, \quad x \geq 0.$$

Hence the effective Hamiltonian

$$H_\lambda(\gamma) = -\frac{\hbar^2}{2m_e} \Delta + V_\lambda^{(\gamma)}, \quad \lambda > 0,$$

takes the form

$$H_\lambda(\gamma) = H_{\text{hyd}} + W_\lambda^{(\gamma)}.$$

The next theorem follows from a simple application of Theorem 4.1:

Theorem 6.1. For all $\lambda > 0$ and $\gamma > 0$, $H_\lambda(\gamma)$ is self-adjoint with $D(H_\lambda(\gamma)) = D(\Delta)$ and bounded below. Moreover, $\sigma_{\text{disc}}(H_\lambda(\gamma))$ is infinite and

$$\sigma_{\text{disc}}(H_\lambda(\gamma)) \subset (-\infty, 0), \quad \sigma_{\text{ess}}(H_\lambda(\gamma)) = [0, \infty).$$

We take $r_n > 0$ such that $r_n < |E_{n+1} - E_n|$ and set

$$C_{r_n}(E_n) := \{z \in \mathbb{C} \mid |z - E_n| = r_n\}.$$

Let

$$M_n := r_n \sup_{z \in C_{r_n}(E_n)} \|H(\gamma) - z\|^{-1}, \quad R_{\lambda,n} := \sup_{z \in C_{r_n}(E_n)} \|W_\lambda^{(\gamma)}(H(\gamma) - z)^{-1}\|.$$

We denote by $H_\lambda^{\ell,s}(\gamma)$ the reduced part of $H_\lambda(\gamma)$ to \mathcal{H}_ℓ^s .

We have from Corollary 5.1 the following result:

Theorem 6.2. Let $n \in \mathbb{N}$, $\ell = 0, 1, \dots, n-1$ and $s = -\ell, -\ell+1, \dots, \ell$. Suppose that $\lambda > 0$ and $R_{\lambda,n} < 1/(1 + M_n)$. Then, $H_\lambda^{\ell,s}(\gamma)$ has a unique simple eigenvalue $E_{n,\ell,s}(\lambda)$ near E_n with

$$E_{n,\ell,s}(\lambda) = E_n + \frac{\left\langle \psi_{n,\ell,s}, W_\lambda^{(\gamma)} \psi_{n,\ell,s} \right\rangle + \sum_{p=1}^{\infty} F_{n,\ell,s}^{(p)}(\lambda)}{1 + \sum_{p=1}^{\infty} G_{n,\ell,s}^{(p)}(\lambda)},$$

where

$$F_{n,\ell,s}^{(p)}(\lambda) := \frac{(-1)^{p+1}}{2\pi i} \int_{C_{r_n}(E_n)} \left\langle \psi_{n,\ell,s}, \left[W_\lambda^{(\gamma)}(H(\gamma) - z)^{-1} \right]^{p+1} \psi_{n,\ell,s} \right\rangle dz,$$

$$G_{n,\ell,s}^{(p)}(\lambda) := \frac{(-1)^{p+1}}{2\pi i} \int_{C_{r_n}(E_n)} \frac{\left\langle \psi_{n,\ell,s}, \left[W_\lambda^{(\gamma)}(H(\gamma) - z)^{-1} \right]^p \psi_{n,\ell,s} \right\rangle}{E_n - z} dz.$$

Moreover, a normalized eigenvector $\psi_{n,\ell,s}^{(\lambda)}$ of $H_\lambda^{\ell,s}(\gamma)$ with eigenvalue $E_{n,\ell,s}(\lambda)$ is given by

$$\psi_{n,\ell,s}^{(\lambda)} = \frac{\psi_{n,\ell,s} + \sum_{p=1}^{\infty} S_{n,\ell,s}^{(p)}(\lambda)}{\sqrt{1 + \sum_{p=1}^{\infty} G_{n,\ell,s}^{(p)}(\lambda)}},$$

where

$$S_{n,\ell,s}^{(p)}(\lambda) := \frac{(-1)^{p+1}}{2\pi i} \int_{C_{r_n}(E_n)} (H(\gamma) - z)^{-1} \left[W_\lambda^{(\gamma)}(H(\gamma) - z)^{-1} \right]^p \psi_{n,\ell,s} dz.$$

Let $n \in \mathbb{N}$, $\lambda > 0$ and $R_{\lambda,n} < 1/(1 + M_n)$. Then, by Theorem 6.2, one can define

$$(6.2) \quad \Delta E_n(\ell, s; \ell', s') := E_{n,\ell,s}(\lambda) - E_{n,\ell',s'}(\lambda)$$

for $\ell, \ell' = 0, 1, \dots, n-1$, $s, s' = -\ell, -\ell+1, \dots, \ell$ with $(\ell, s) \neq (\ell', s')$. We call it an energy level shift of $H_\lambda(\gamma)$ with respect to the n -th energy level.

The next theorem is an important result necessary for deriving the Lamb shift (see the next section):

Theorem 6.3. Under the assumption of Theorem 6.2, the following holds:

$$(6.3) \quad E_{n,\ell,s}(\lambda) = E_n + 4\pi\gamma |\psi_{n,\ell,s}(\mathbf{0})|^2 \lambda + o(\lambda) \quad (\lambda \rightarrow 0).$$

§ 7. Derivation of the Lamb Shift

In this section, we assume that, for each $n \in \mathbb{N}$, $\lambda > 0$ is sufficiently small so that the assumption of Theorem 6.2 holds. Then, by Theorem 6.3, we have

$$\Delta E_n(\ell, s; \ell', s') = 4\pi\gamma(|\psi_{n,\ell,s}(\mathbf{0})|^2 - |\psi_{n,\ell',s'}(\mathbf{0})|^2)\lambda + o(\lambda) \quad (\lambda \rightarrow 0).$$

Using

$$L_n^1(0) = nn!, \quad Y_0^0 = \frac{1}{\sqrt{4\pi}},$$

we obtain

$$(7.1) \quad |\psi_{n,\ell,s}(\mathbf{0})|^2 = \begin{cases} \frac{1}{\pi} \left(\frac{m_e \gamma}{\hbar^2} \right)^3 \frac{1}{n^3}; & \ell = 0, s = 0 \\ 0 & ; \ell \geq 1 \end{cases}$$

Hence the following hold:

(i) If $\ell, \ell' \geq 1$, then

$$(7.2) \quad \Delta E_n(\ell, s; \ell', s') = o(\lambda) \quad (\lambda \rightarrow 0).$$

(ii) If $\ell \geq 1$, then

$$(7.3) \quad \Delta E_n(0, 0; \ell, s) = 4\pi\gamma\lambda|\psi_{n,0,0}(\mathbf{0})|^2 + o(\lambda) \quad (\lambda \rightarrow 0).$$

Formula (7.3) shows that, for each n , the energy of the state with $\ell = 0, s = 0$ (the s -state) is higher than that of the state with $\ell \geq 1$ for all sufficiently small λ . This may be a non-relativistic correspondence of the experimental fact that, for $n = 2$, the energy of the state $2s_{1/2}$ is higher than that of the state $2p_{1/2}$.

To compare the value of $\Delta E_n(0, 0; \ell, s)$ with the experimental one, we take $\lambda = \lambda_q$ with $q = -e$, $m = m_e$ and

$$\omega(\mathbf{k}) = |\mathbf{k}|, \quad \hat{\rho}(\mathbf{k}) = \frac{1}{\sqrt{(2\pi)^3}} \chi_{[\omega_{\min}/\hbar c, \omega_{\max}/\hbar c]}(|\mathbf{k}|), \quad \mathbf{k} \in \mathbb{R}^3,$$

with constants $\omega_{\min} > 0$ and $\omega_{\max} > 0$ satisfying $\omega_{\min} < \omega_{\max}$. Then we have

$$\lambda = \lambda_{-e} = \alpha \left(\frac{\hbar}{m_e c} \right)^2 \frac{1}{3\pi} \log \frac{\omega_{\max}}{\omega_{\min}},$$

where

$$\alpha := \frac{e^2}{4\pi\hbar c} \approx \frac{1}{137}$$

is the fine structure constant. We remark that ω_{\min} (resp. ω_{\max}) physically means an infrared (resp. ultraviolet) cutoff of the one-photon energy. We have $\gamma = Ze^2/4\pi$. Thus we obtain

$$(7.4) \quad \begin{aligned} \Delta E_n(0, 0; \ell, s) &\approx \alpha^5 \frac{4}{3\pi} m_e c^2 \frac{Z^4}{n^3} \log \frac{\omega_{\max}}{\omega_{\min}} \\ &= \frac{8}{3\pi} \alpha^3 \text{Ry} \frac{Z^4}{n^3} \log \frac{\omega_{\max}}{\omega_{\min}} \quad (\alpha \rightarrow 0), \end{aligned}$$

where $\text{Ry} := \alpha^2 m_e c^2 / 2$ is 1 rydberg ($-\text{Ry}$ is the ground state energy of the hydrogen atom). If we take $\omega_{\max} = m_e c^2$ (the rest mass energy of the electron) and $\omega_{\min} = 17.8 \text{ Ry}$, then the right hand side of (7.4) completely coincides with Bethe's calculation [8] of the Lamb shift. Hence it is in a good agreement with the experimental result.

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